The embodiments of the invention in which an exclusive property or privilege is claimed are defined as follows:

- 1. A method for discovering new compounds with expression profilealtering activity, comprising:
- (a) determining a first expression profile of a set of representative molecules in a first biological sample;
- (b) determining a second expression profile of the set of molecules in a second biological sample, wherein the second biological sample differs from the first biological sample by a known parameter;
- (c) determining a third expression profile of the set of molecules in the second biological sample after treatment of the second biological sample with at least one analyte of previously uncharacterized specific pharmacological activity; and
- (d) comparing the third expression profile with the first and second expression profiles to identify one or more analytes that induces a third expression profile that is more similar to the first expression profile than is the second expression profile.
 - 2. The method of Claim 1, wherein step (d) comprises:
- (a) deriving a first difference profile by comparing the first expression profile with the second expression profile;
- (b) deriving a second difference profile by comparing the second expression profile with the third expression profile; and
- (c) comparing the first difference profile with the second difference profile to identify one or more candidate analytes.
- 3. The method of Claim 1, wherein step (d) is accomplished by using neural network computing to classify expression profiles.
- 4. The method of Claim 1, wherein at least one of the expression profiles is determined using serial analysis of gene expression.

- 5. The method of Claim 1, wherein the expression profile of step (a) or (b) is derived from publicly available literature or data.
- 6. The method of Claim 1, wherein the first or second biological sample is selected from one or more of the group of a specific cell type in vitro, a combination of cell types in vitro, a specific tissue type in vitro, a combination of tissue types in vitro, organs in vitro, a specific cell type in vivo, a combination of cell types in vivo, a specific tissue type in vivo, a combination of tissue types in vivo, organs in vivo, and an entire single-celled or multicellular organism.
- 7. The method of Claim 1, wherein at least one biological sample is derived from a disease state.
- 8. The method of Claim 1, wherein the representative molecules are selected from the group of mRNA transcripts or cDNA derived therefrom, proteins, phosphoproteins, carbohydrates, and lipids.
- 9. The method of Claim 1, wherein at least one of the expression profiles of molecules is determined using polynucleic acid microarrays.
- 10. The method of Claim 9, wherein the polynucleic acid microarrays differentially bind specific peptides.
- 11. The method of Claim 1, wherein at least one of the expression profiles is determined by simultaneously detecting the rates of transcriptions of multiple genes.
- 12. The method of Claim 1, wherein at least one of the expression profiles of molecules is determined using capillary electrophoresis.
- 13. The method of Claim 1, wherein at least one of the expression profiles of molecules is determined using 2-dimensional gel electrophoreses.

- 14. The method of Claim 1, wherein at least one of the expression profiles of molecules is determined by using antibody arrays.
- 15. The method of Claim 1, wherein at least one of the expression profiles of molecules is determined by using spectrometry techniques.
- 16. The method of Claim 15, wherein the spectrometry technique is mass spectrometry.
- 17. The method of Claim 1, wherein at least one of the expression profiles of molecules is determined by using a method selected from the group consisting of, fiber-optic, bead-based mRNA and protein detection.
- 18. The method of Claim 1, wherein at least one of the expression profiles is determined using differential display.
- 19. The method of Claim 1, wherein step (c) is conducted many times in high-throughput fashion with analytes from a library of analytes with previously uncharacterized activity relative to the parameter by which the first and second samples are known to differ.
- 20. The method of Claim 1, wherein the first expression profile of step (a) is derived from a combination of biological samples or sources of data.
- 21. The method of Claim 1, wherein the tested analyte of step (c) possesses previously characterized pharmacological activity unrelated to the parameter by which the first and second biological samples are known to differ, and where its pharmacological activity relative to said parameter is previously uncharacterized.
- 22. The method of Claim 1, wherein the expression profile of molecules is determined by using chromatographic techniques.

- 23. The method of Claim 22, wherein the chromatographic technique is HPLC.
- 24. The method of Claim 22, wherein the chromatographic technique is gas chromatography.
- 25. The method of Claim 1, wherein the expression profile of molecules is determined using Western blot.